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# Some recent developments in the modelling of crack growth in ceramics with transformation behaviour

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The dilatant transformation model developed by McMeeking and Evans<sup>1</sup> is extended for two applications. First, the effect on toughness of inhomogeneous distributions of tetragonal zirconia particles is investigated. Second, the shear component of the  $t \rightarrow m$  transformation is taken into account and the effects on the shape and magnitude of the transformation zone and the toughness are determined. Both problems are investigated using numerical analysis to determine the development of the transformation zone and the toughness during mode I crack growth.

**Keywords:** transformation mode; crack growth; ceramics

The stress-induced (martensitic-like) transformation of zirconia from a tetragonal to a monoclinic structure ( $t \rightarrow m$ ) may give rise to substantial toughening of ceramics. This toughening mechanism has been applied in partially stabilized zirconia (PSZ), tetragonal zirconia polycrystal (TZP) and zirconia toughened alumina (ZTA). The first modelling was performed by McMeeking and Evans<sup>1</sup> and Budiansky *et al.*<sup>2</sup>. This model significantly enlarged the understanding of transformation toughening but there was unsatisfactory quantitative agreement. Here we present two issues which may result in a better agreement. First, we will treat the effect of inhomogeneous distributions of  $t$ -zirconia in ZTA due to processing. Second, we will consider an extension to the above dilatation model<sup>1,2</sup> to account for shear strains. Plane strain will be assumed throughout the paper.

## Effects of clustering

During the forming process, fine-grained powders tend to agglomerate<sup>3</sup>, which, during sintering, causes inhomogeneities in the distribution of  $\text{ZrO}_2$ . These inhomogeneities have been avoided as much as possible, since they were believed to lower the toughness. In our analysis, we will consider ZTA materials with a large tetragonal fraction of the total  $\text{ZrO}_2$  content. In these materials the transformation toughening mechanism is generally considered to dominate completely over the microcrack mechanism, and in the further analysis we will neglect the contribution of microcrack toughening.

The  $t \rightarrow m$  transformation of an isolated  $\text{ZrO}_2$  particle, which is triggered by a sufficiently high stress, is accompanied by a volume increase of about 4.5% and a shear strain of 16%. The model proposed in references 1 and 2 only takes into account the dilatation  $\theta$ , as the average shear strain is assumed to be very small due to twinning, when the particle is embedded in a matrix. The onset of the transformation is assumed to occur at a critical mean stress  $\sigma_m^c$ , as shown in Figure 2, and the value  $\bar{B}$  of the bulk modulus of the intermediate segment of the dilatant stress-strain curve determines whether the transformation continues spontaneously and immediately to completion (a so-called supercritical transformation, characterized by  $\bar{B} < -4G/3$ , where  $G$  is the shear modulus) or gradually. In the latter case the material can remain stable in a state in which only part of the particles are transformed (a so-called subcritical transformation

which occurs as  $\bar{B} > -4G/3$ ). Finally, the solution depends on the strength of the transformation which is characterized by the non-dimensional parameter  $\omega = (E\theta^T/\sigma_m^c)(1 + \nu)/(1 - \nu)$ . Here, the maximum transformation dilatation is  $\theta^T = c\theta_p^T$ , where  $c$  is the volume fraction of  $t$ - $\text{ZrO}_2$  particles and  $\theta_p^T$  the maximum transformation dilatation in each particle ( $\theta_p^T \approx 4.5\%$ ).

The numerical solution scheme we use is similar to the one described by Hom and McMeeking<sup>4</sup>. A large semi-circular region around the crack tip is considered, with boundary conditions according to the usual far-field solution corresponding to an applied stress intensity  $K^{\text{APP}}$  (see Figure 1). During crack growth  $K^{\text{APP}}$  was adjusted to maintain the near-tip stress intensity  $K^{\text{TIP}} = K^C$ , with  $K^C$  the fracture toughness of the material. Results from calculations with homogeneously distributed  $\text{ZrO}_2$  were in agreement with those in reference 4. Here and in the following all lengths will be normalized by  $L = 2/(9\pi)[K_1^c\{h_0(1 - 2\nu) + (1 + \nu)\}/(\Sigma_c)]^2$ , where  $h_0$  and the critical stress  $\Sigma_c = C_0(\theta, f)/(3\varepsilon^{\text{pd}})$  will be defined later. For this model, with  $\theta^T = 3\varepsilon^{\text{pd}}$ , it follows that  $\Sigma_c = \sigma_m^c$  and  $h_0 = 0$ . Physically,  $L$  is the distance from the crack tip ahead to the boundary of the transformation zone when the transformation strains go to zero and do not disturb the stress distribution.

To model the inhomogeneous distribution of  $t$ - $\text{ZrO}_2$  particles an area function  $D(x, y)$  is introduced, such that

$$\theta^T = D(x, y)c\theta_p^T \text{ and } D(x, y) = 1 + a \cos\left(\frac{\pi x}{2L^c}\right) \cos\left(\frac{\pi y}{2L^c}\right) \quad (1)$$

where  $a \in [0, 1]$  is a parameter which adjusts the strength of the inhomogeneity and  $L^c$  defines the length scale of the inhomogeneities. For the calculations, we have used Poisson's ratio  $\nu = 0.3$ ,  $\bar{B}/G = 0$ ,  $a = 1$  and  $\omega = 5$ . Three different values for  $L^c$  were chosen, namely 0.5 $L$ ,  $L$  and 4 $L$ , which correspond to inhomogeneities in the order of the transformation zone height. Crack growth was forced to follow path A, shown in Figure 3. The results, plotted in Figure 4, show an increased toughening compared to results for homogeneous distribution. It must be noted that the ratio  $K^{\text{APP}}/K^{\text{TIP}}$  is oscillating during growth and it is assumed that the crack grows as long as  $K^{\text{TIP}} > K^C$ . From this point of view the horizontal parts in the resistance curves must be seen as unstable

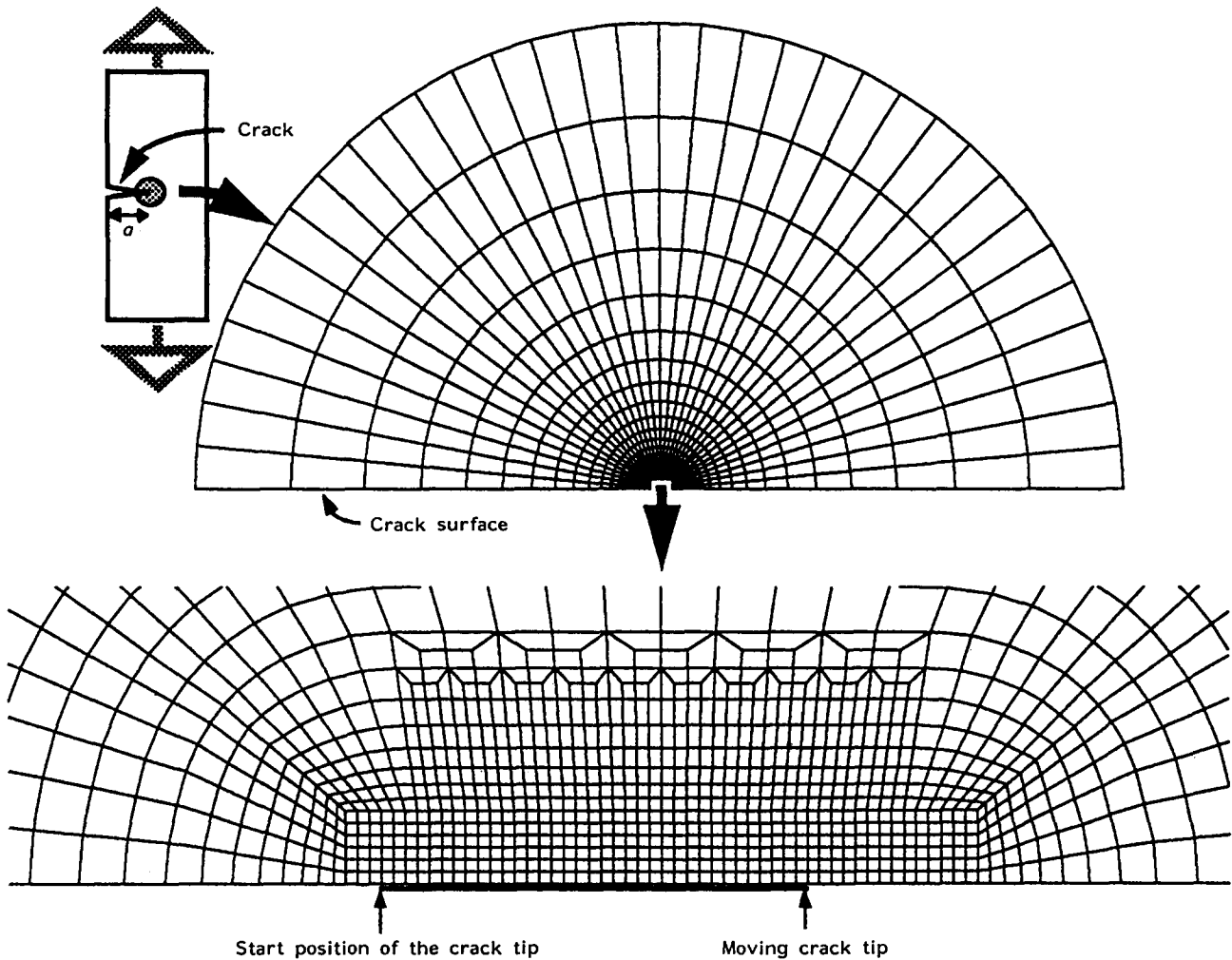


Figure 1 The finite-element mesh used for crack-growth calculations. The number of elements in the radial direction is equal to 40

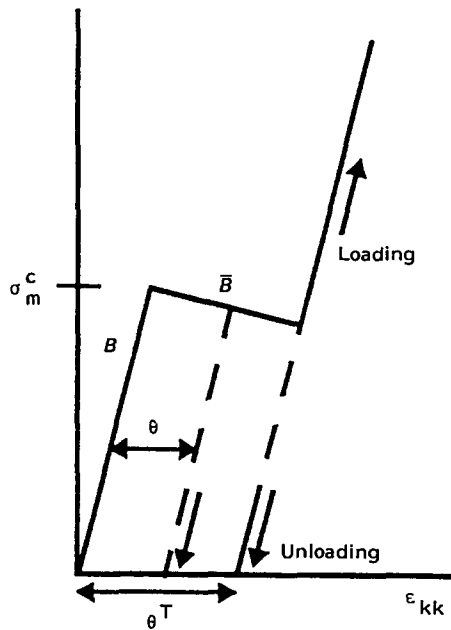


Figure 2 Material behaviour for material with dilatant transformation strains

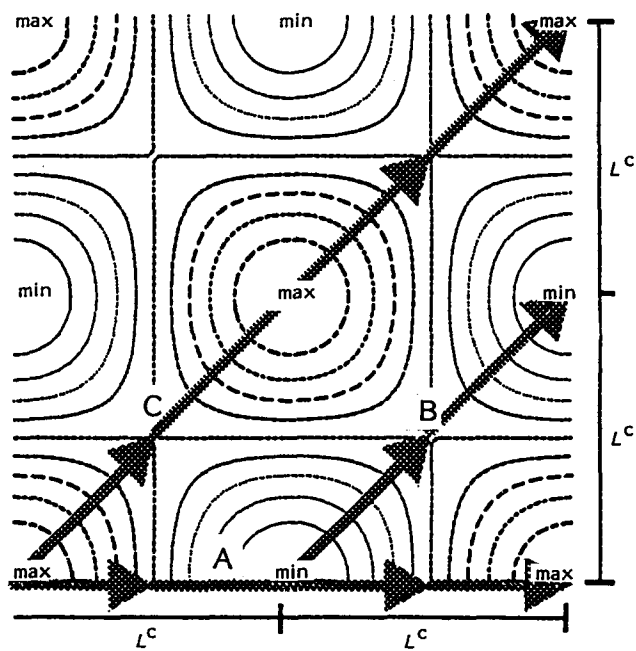
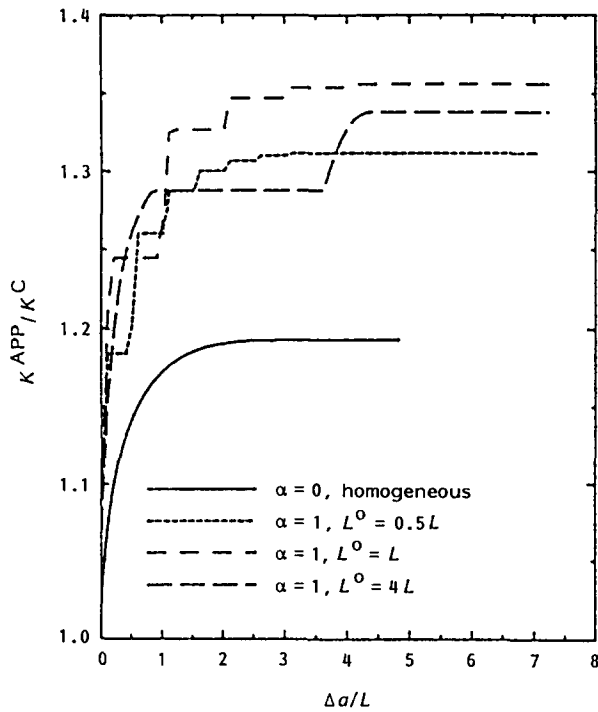


Figure 3 Schematic representation of the inhomogeneities. Crack directions A, B and C are indicated

and the crack jumps from one oscillation to another. It is seen that a decreasing value of  $L^c$  results in a decreasing toughness increment, and in the limit the distribution

becomes homogeneous. It must be noted that for the case with  $L^c = 4L$  the steady-state value has not yet been reached. When crack growth was forced to follow the



**Figure 4** Toughness development during crack growth in inhomogeneous materials

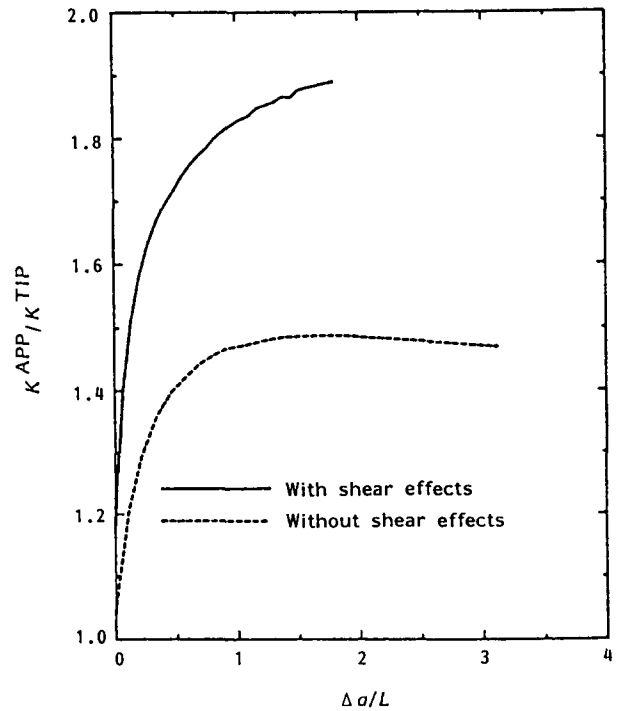
diagonal paths B or C (Figure 3) a lower steady-state value for the toughness was found of, respectively, about 5% and 2.5%.

From these kinds of numerical calculations it can be concluded that inhomogeneities may give rise to an increase in toughness compared to materials with a perfectly homogeneous distribution of  $\text{ZrO}_2$ . This might explain the development of duplex materials where relatively large (10–50  $\mu\text{m}$ ) spherical  $t\text{-ZrO}_2$  particles are dispersed in a ceramic matrix.

### Shear effects of the transformation

The shear strains associated with the  $t \rightarrow m$  transformation have long been neglected as they were assumed to be small due to twinning. However, work of Lambropoulos<sup>5</sup> revealed that the influence on the shape of the transformation zone can be quite substantial and an enhanced toughening increment could be found, which was in better agreement with experiments. In 1986, Chen and Reyes Morel<sup>6</sup> published results of hydraulic compression experiments which showed shear and dilatation effects of comparable magnitude. Based on references 5 and 6, Sun *et al.*<sup>7</sup> developed a new micromechanics-based model. Here, we adopt this model to account for the shear effects and the influence on toughening during crack growth.

In the derivation of the transformation plasticity model, Sun *et al.*<sup>7</sup> assume the continuum element to consist of a large number of transformable inclusions (referred to by I) embedded coherently in an elastic matrix (referred to by M). Microscopic quantities (in the continuum element) will be referred to by lower-case letters. The macroscopic quantities can be found by taking the volume average  $\langle \rangle$  of the microscopic quantities over the element. Continuum strain can then be split into an elastic and a plastic part due to the transformation, and the incremental macroscopic plastic strain is then given by  $d\mathbf{E}^p = d\mathbf{E}^{pd} + d\mathbf{E}^{ps} = \langle \mathbf{E}^{pd} \rangle_{dV_I} df + \langle \mathbf{E}^{ps} \rangle_{dV_I} df$ ,



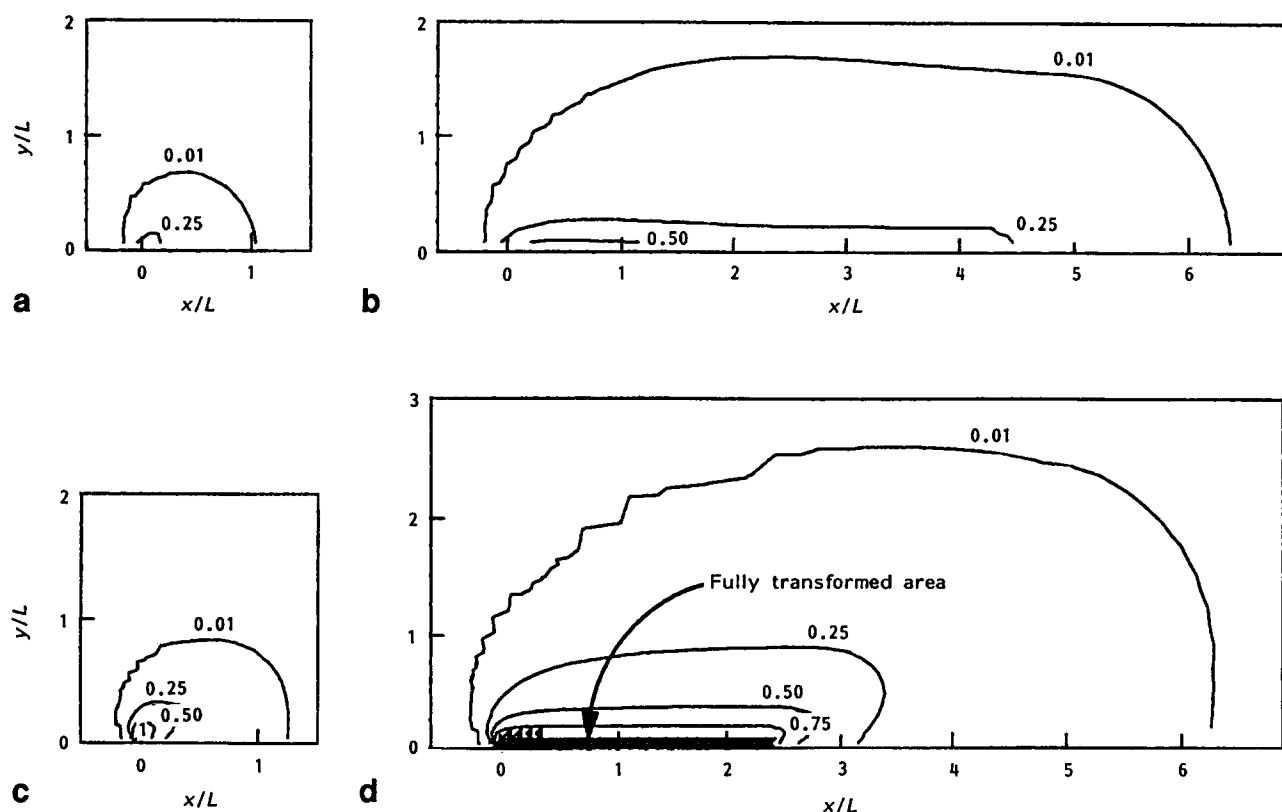
**Figure 5** Toughness development when the shear effects are taken into account and when only dilatation is considered

where  $\langle \mathbf{E}^{pd} \rangle_{dV_I} = \mathbf{E}^{pd}$  is the dilatation which is about 1.5% at room temperature and  $\langle \mathbf{E}^{ps} \rangle_{dV_I} = A(s_{ij}^M/\sigma_c^M)$ , where  $A$  is a material parameter,  $s_{ij}^M$  is the average deviatoric stress in the matrix and the von Mises stress  $\sigma_c^M = [(3/2)s_{ij}^M s_{ij}^M]^{1/2}$ . The forward transformation yielding function can now be written as

$$F_1(\sigma, f, \theta, \langle \mathbf{E}^{ps} \rangle_{dV_I}) = \frac{2}{3} A \sigma_c^M + 3 \mathbf{E}^{pd} \sigma_m^M - C_0(\theta, f) \quad (2)$$

where  $C_0(\theta, f)$  is a term which takes into account the contribution of energy change due to differences in surface energy, free chemical energy and dissipation due to interface friction. Finally, the measure of dependency of  $C_0(\theta, f)$  on  $f$ , to be able to describe hardening, is governed by a parameter  $\alpha$ . For PSZ materials Sun *et al.*<sup>7</sup> estimated  $\alpha = 1.2$ ,  $h_0 = 1.3$  ( $h_0 = A/(3\mathbf{E}^{pd})$ ),  $\nu = 0.3$  and  $f = 0.35$ . For a uniaxial tensile experiment it was found that the tangent of the plastic branch was equal to  $0.1E$ , with  $E = 208$  GPa. The stress level at which transformation plasticity develops was estimated to be  $\Sigma_{II} = 530$  MPa. Based on these input parameters, a crack growth calculation has been performed and the results are shown in Figures 5 and 6. For comparison, a second computation has been performed where the shear effect was not included. The value of the parameter  $\alpha$  has been estimated in that case such that the above-mentioned tangent of the plastic branch in the tensile experiment is maintained.

From Figure 6 we see the shape of the transformation zone to be different when the shear effects are taken into account. It is found that the shear and dilatation strains are of comparable magnitude. The effect of these differences on the toughness is shown in Figure 5 where the toughness increment is plotted against the crack extension. It can be seen that after considerable crack extension,



**Figure 6** The shape of the transformation zones when only dilatation is considered ((a) and (b)) and when transformation shear strains are also taken into account ((c) and (d)). The initial zones are shown in (a) and (c). Contours are plotted for  $(f_{\epsilon^{pd}})/f_{\max \epsilon^{pd}}$

sion the toughness is increased with a factor 1.9 while a steady-state value has not been reached yet. This must be compared to an increase of about 1.5 when only dilatant transformation is considered. It is noted that calculations with a more refined mesh showed an initial decrease in toughening. However, after some crack growth the decrease converts to an increase in toughness which slightly exceeds the onset of the *R*-curve of Figure 5. More computations will be necessary to clarify these issues. This single example, however, suggests a better quantitative agreement with experiments and research will be continued to increase insights into the problem.

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